

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
 Data File : BP008160.D
 Acq On : 30 Nov 2021 16:08
 Operator : CG/JU
 Sample : M4848-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PSC124055

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.011	3	4	9	rVB	1117118	891541	25.39%	3.445%
2	3.058	9	12	15	rVB	46119	50964	1.45%	0.197%
3	4.928	324	330	338	rBV	203199	282672	8.05%	1.092%
4	5.393	401	409	421	rBV	1713977	2444063	69.60%	9.444%
5	6.987	671	680	694	rBV	1490570	2488348	70.87%	9.615%
6	7.799	811	818	827	rBV	367034	589561	16.79%	2.278%
7	8.963	1007	1016	1030	rBV	968156	1613382	45.95%	6.234%
8	10.399	1254	1260	1275	rBV	37635	90440	2.58%	0.349%
9	10.599	1284	1294	1302	rBV	443510	737583	21.01%	2.850%
10	13.069	1707	1714	1729	rBV	1983214	2947837	83.95%	11.391%
11	13.281	1746	1750	1760	rVB2	25704	47114	1.34%	0.182%
12	14.110	1885	1891	1897	rBV3	27924	56357	1.60%	0.218%
13	14.169	1897	1901	1909	rVB2	23022	37174	1.06%	0.144%
14	14.304	1917	1924	1931	rBV3	37180	103659	2.95%	0.401%
15	14.445	1942	1948	1956	rBV	566925	852808	24.29%	3.295%
16	15.257	2075	2086	2093	rBV2	28912	74458	2.12%	0.288%
17	15.945	2196	2203	2211	rBV	1439253	2107500	60.02%	8.144%
18	17.139	2401	2406	2411	rVB	43106	55336	1.58%	0.214%
19	17.210	2411	2418	2422	rBV	617550	944016	26.88%	3.648%
20	17.251	2422	2425	2430	rVB	107909	139549	3.97%	0.539%
21	17.339	2436	2440	2446	rVB2	40105	66315	1.89%	0.256%
22	17.504	2464	2468	2479	rVB3	18184	45364	1.29%	0.175%
23	18.081	2562	2566	2568	rBV	28098	37246	1.06%	0.144%
24	18.104	2568	2570	2573	rBV3	30938	43497	1.24%	0.168%
25	18.269	2593	2598	2601	rBV2	46676	77062	2.19%	0.298%
26	18.304	2601	2604	2608	rVB	28763	36242	1.03%	0.140%
27	19.227	2756	2761	2767	rBV	229949	307465	8.76%	1.188%
28	19.580	2817	2821	2830	rVB	221369	319069	9.09%	1.233%
29	19.780	2849	2855	2860	rBV	2858820	3511346	100.00%	13.568%
30	19.904	2872	2876	2881	rVB2	19217	35582	1.01%	0.137%
31	20.063	2901	2903	2912	rVB2	42873	51460	1.47%	0.199%
32	21.033	3064	3068	3073	rBV3	145497	216920	6.18%	0.838%
33	21.086	3074	3077	3085	rVB2	124930	156300	4.45%	0.604%
34	21.304	3109	3114	3119	rBV	830171	1203007	34.26%	4.649%
35	21.345	3119	3121	3128	rVB	114100	126848	3.61%	0.490%
36	21.427	3130	3135	3148	rVV	1235721	1869734	53.25%	7.225%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.704	3516	3522	3537	rVB2	574488	1221320	34.78%	4.719%
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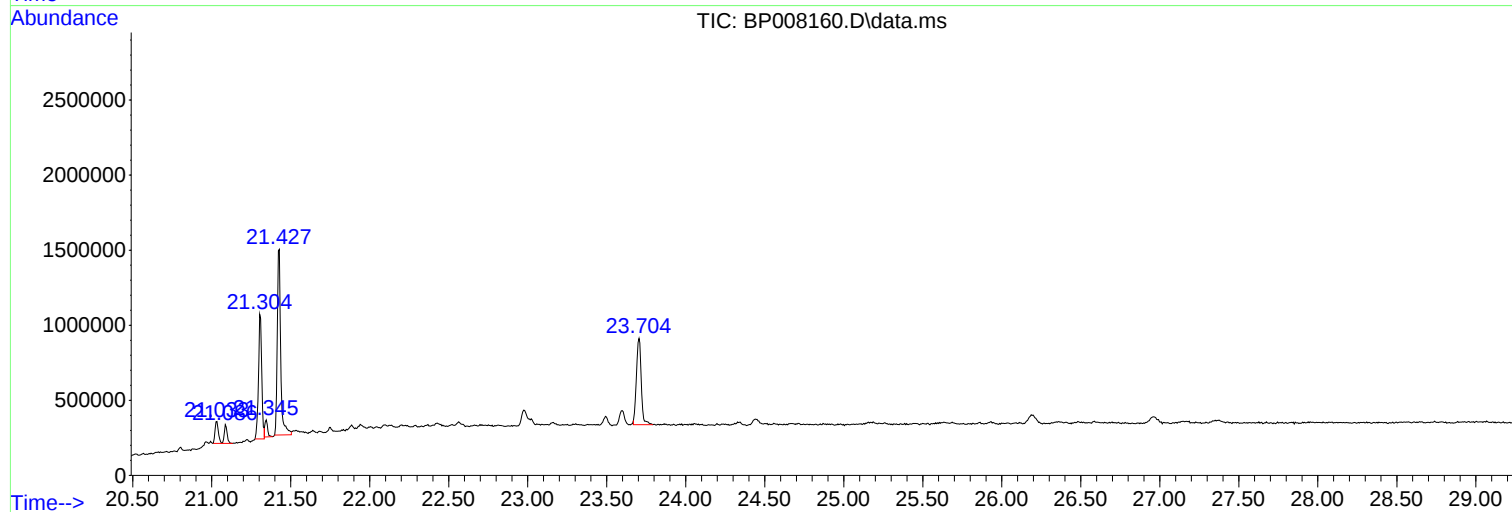
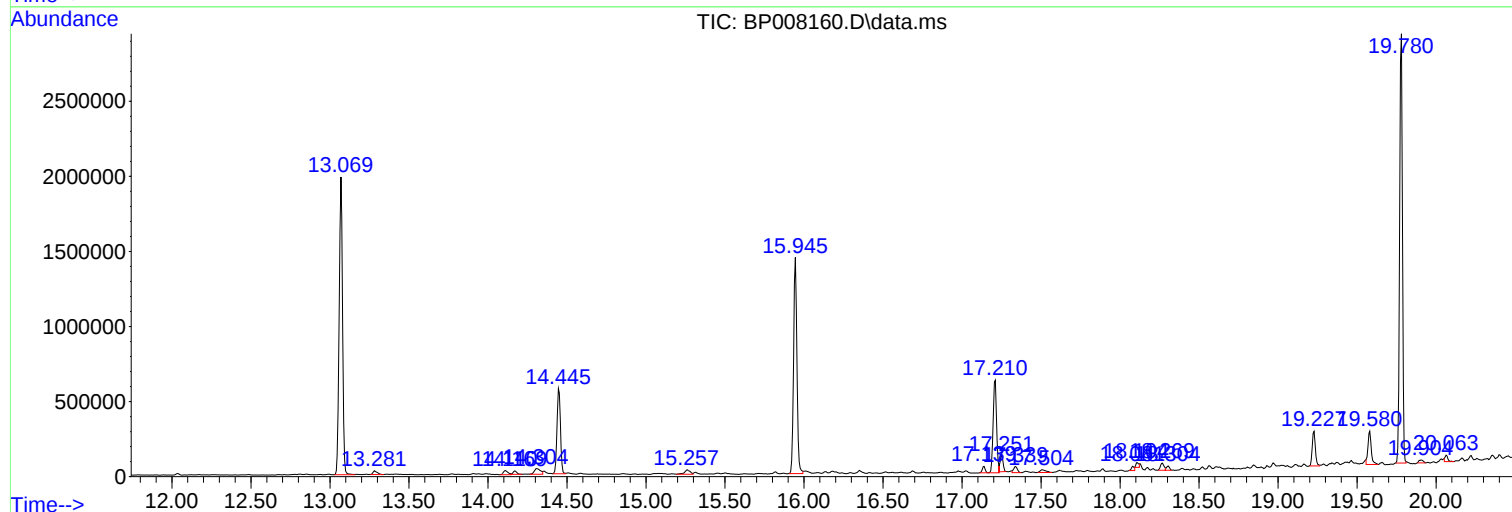
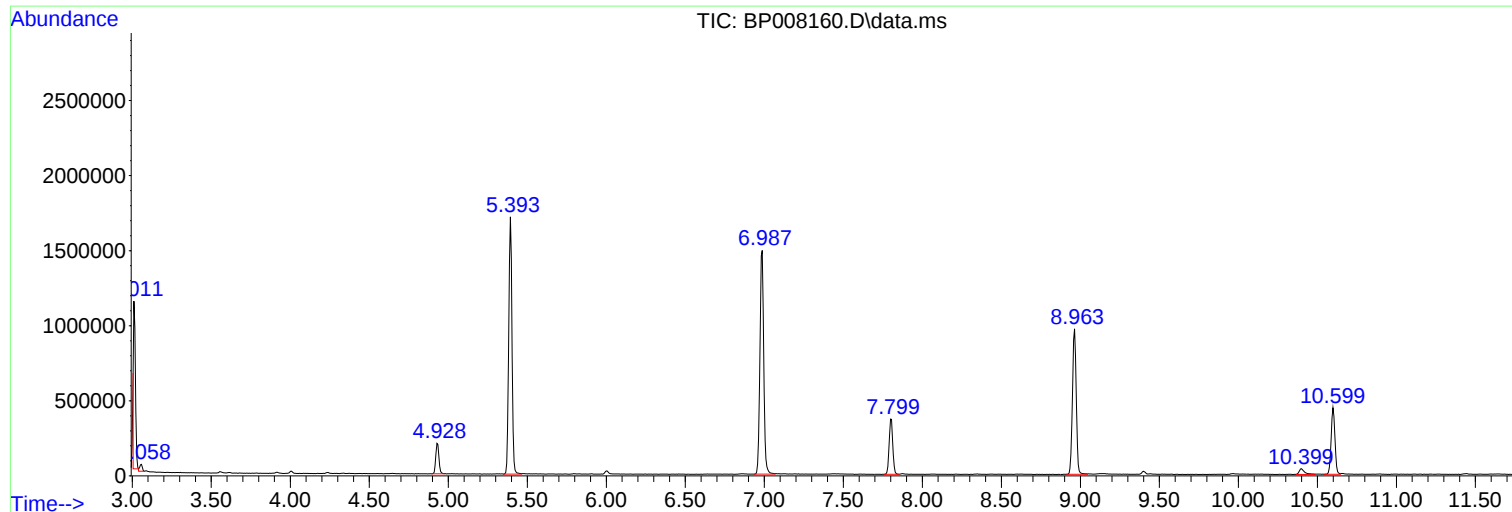
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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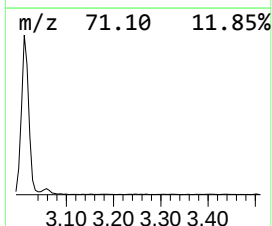
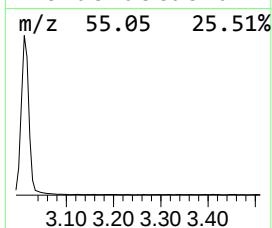
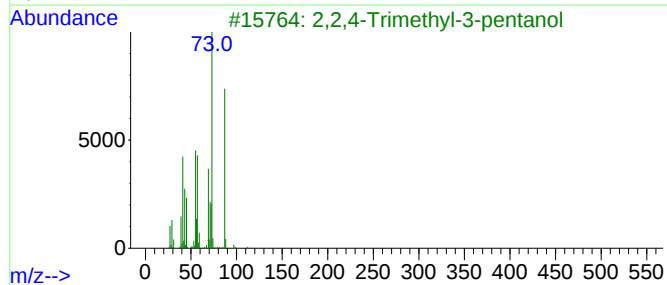
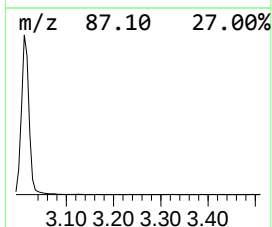
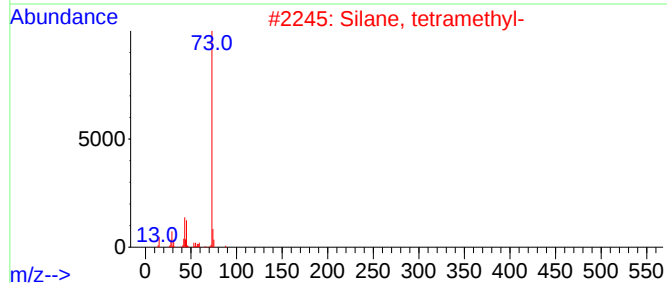
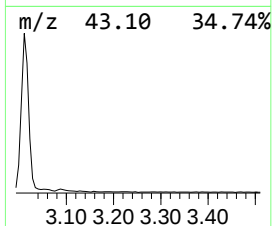
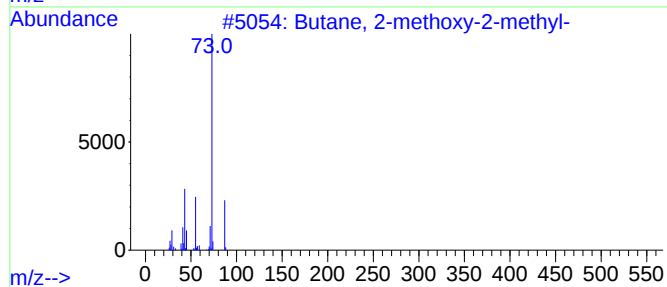
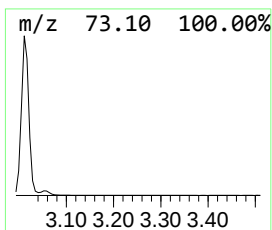
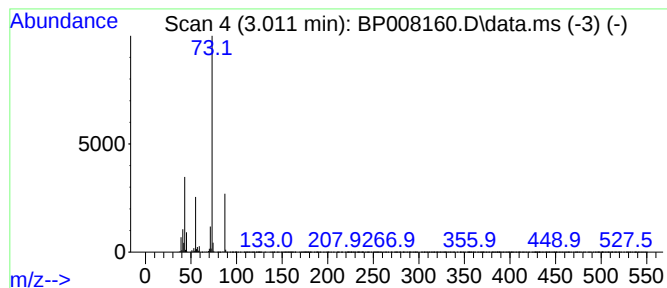
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.011	30.24 ng	891541	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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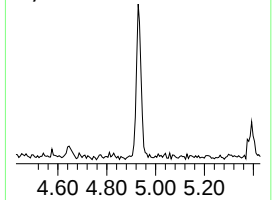
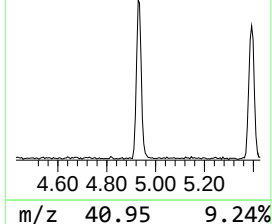
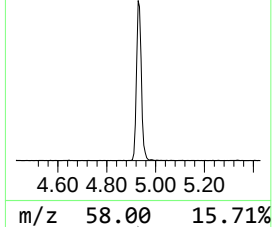
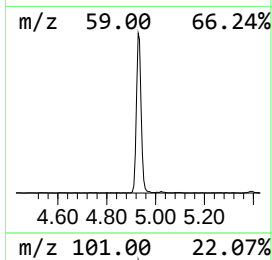
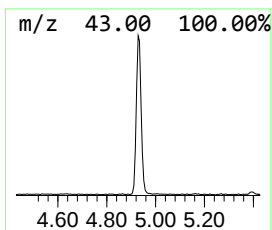
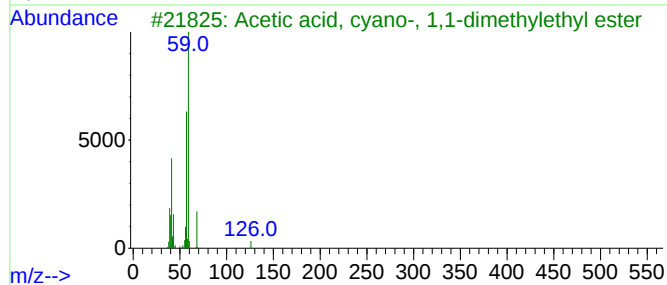
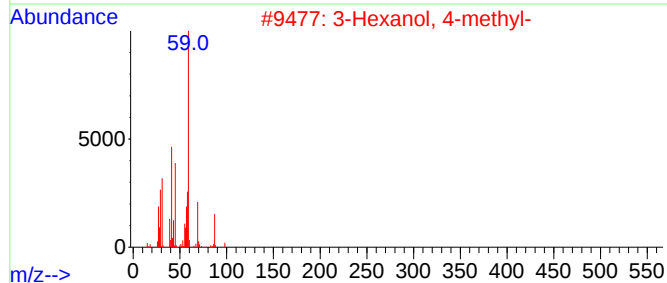
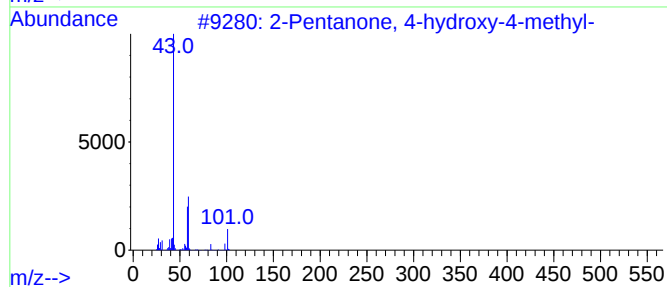
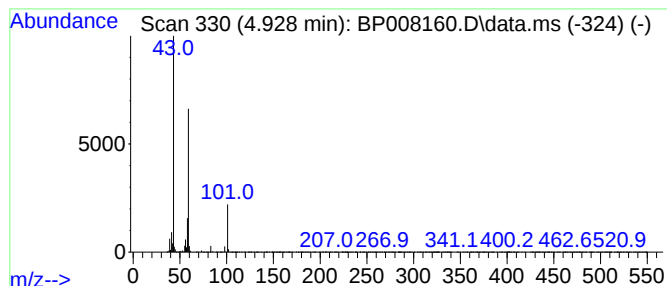
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	9.59 ng	282672	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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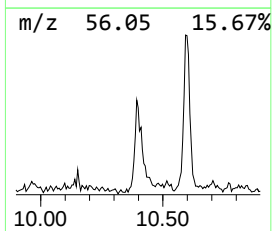
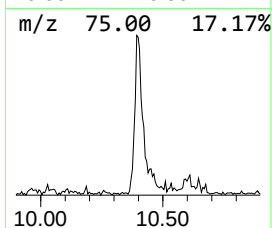
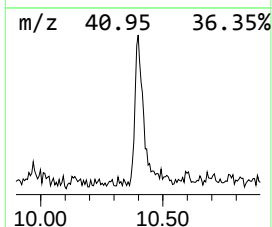
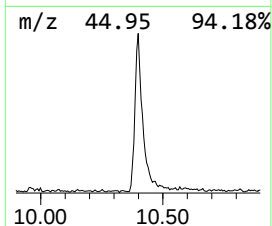
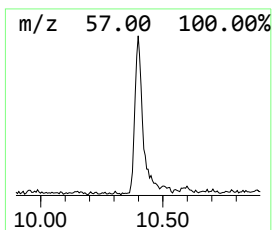
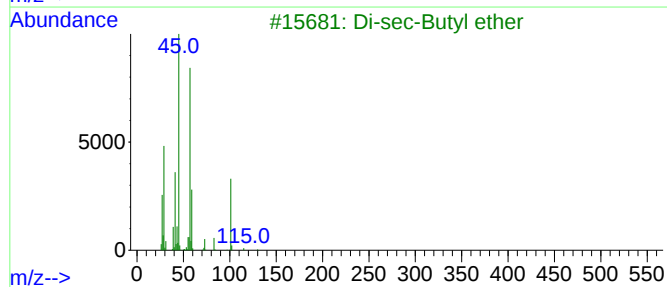
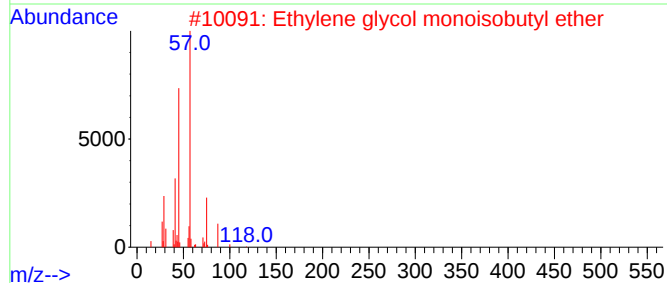
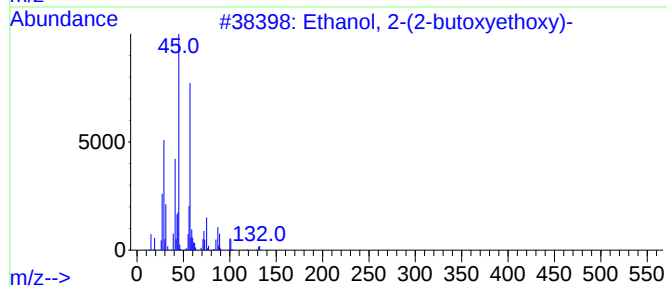
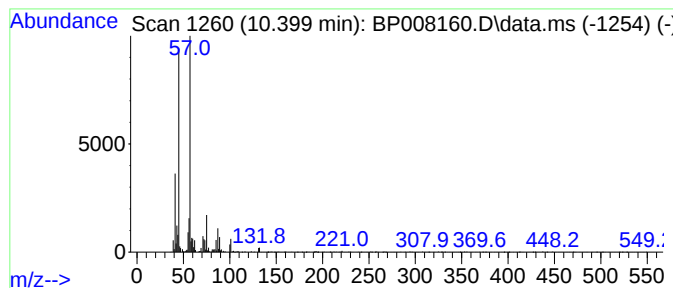
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.399	2.45 ng	90440	Naphthalene-d8	10.599

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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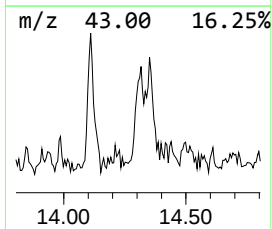
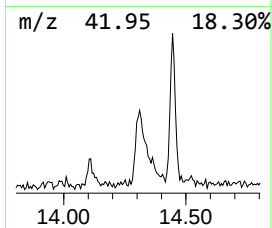
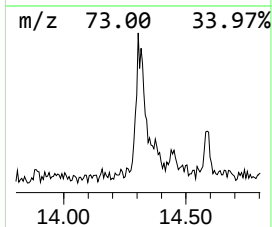
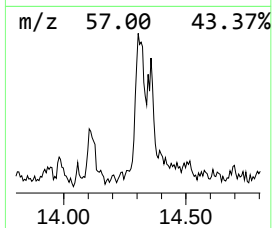
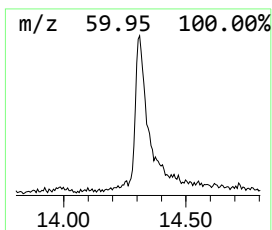
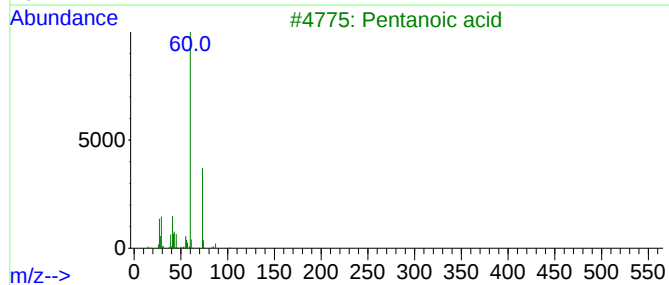
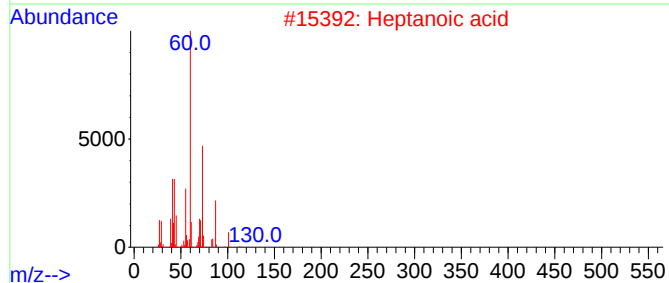
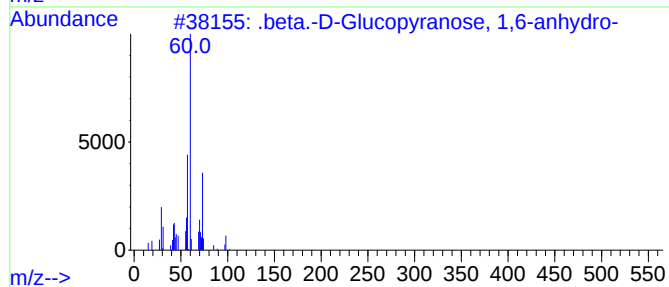
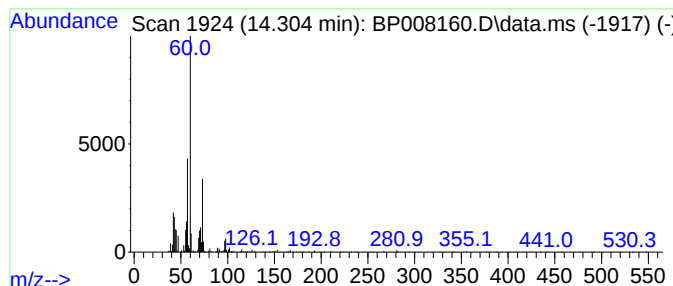
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 .beta.-D-Glucopyranose, 1,6... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.304	2.43 ng	103659	Acenaphthene-d10	14.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	78
2			Heptanoic acid	130	C7H14O2	000111-14-8	64
3			Pentanoic acid	102	C5H10O2	000109-52-4	53
4			Butanoic acid	88	C4H8O2	000107-92-6	53
5			Hexanoic acid	116	C6H12O2	000142-62-1	53



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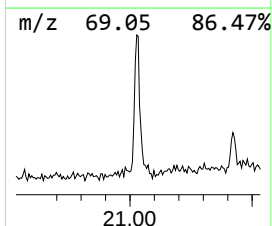
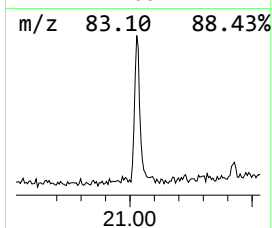
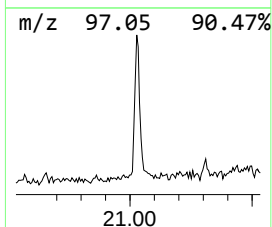
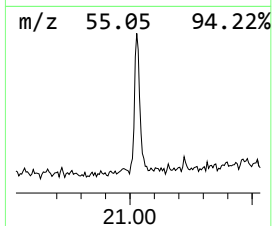
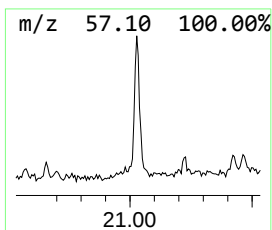
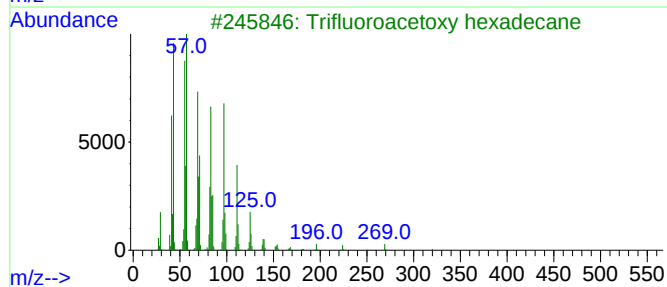
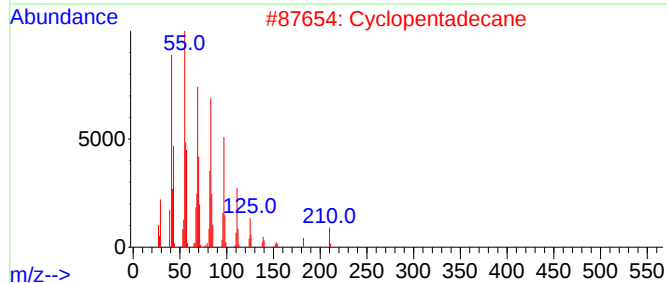
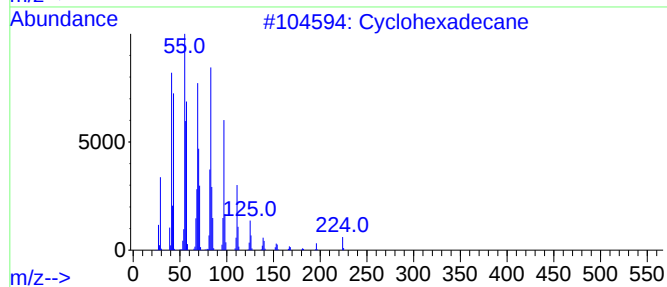
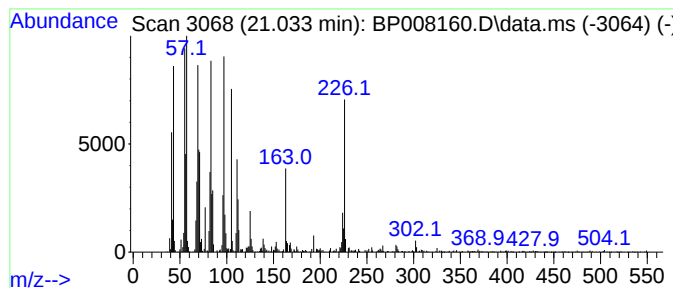
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	3.61 ng	216920	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	93
2			Cyclopentadecane	210	C15H30	000295-48-7	90
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
4			Behenic alcohol	326	C22H46O	000661-19-8	76
5			1-Nonadecene	266	C19H38	018435-45-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008160.D
Acq On : 30 Nov 2021 16:08
Operator : CG/JU
Sample : M4848-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124055

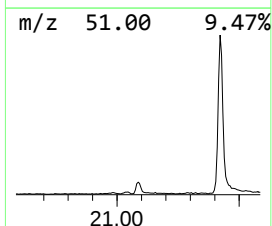
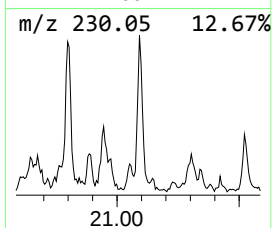
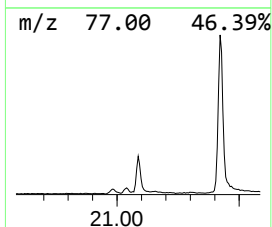
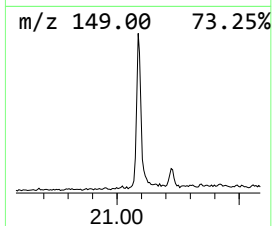
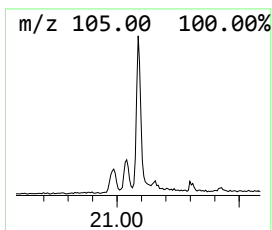
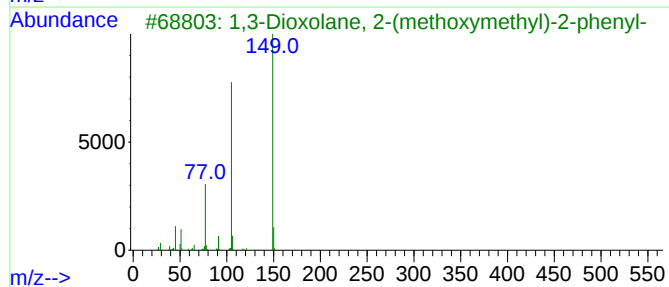
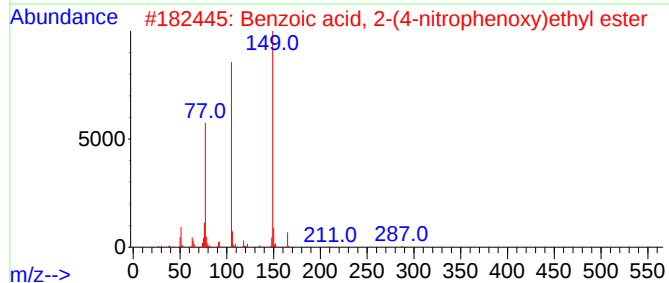
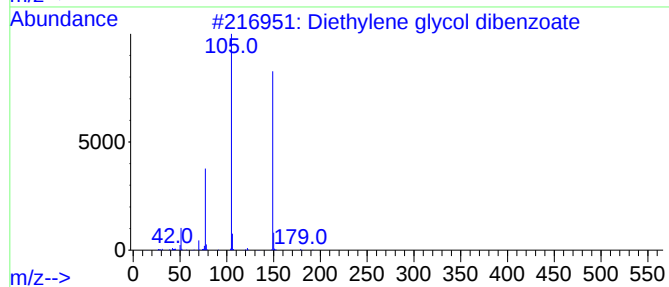
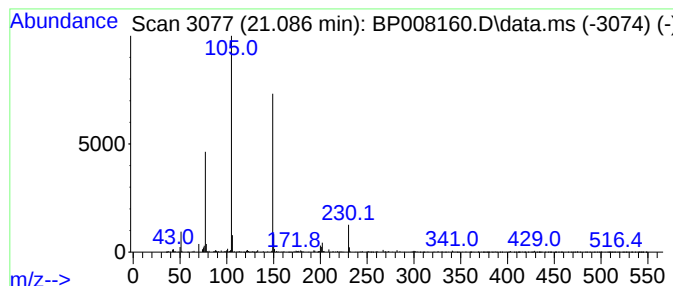
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	2.60 ng	156300	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
4			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	72
5			N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008160.D
Acq On : 30 Nov 2021 16:08
Operator : CG/JU
Sample : M4848-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124055

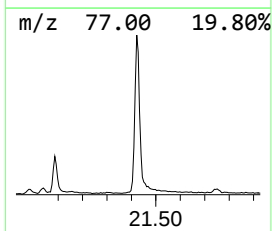
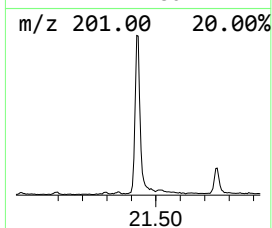
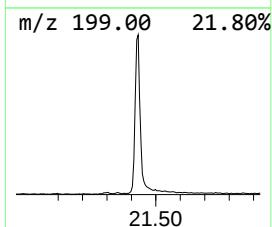
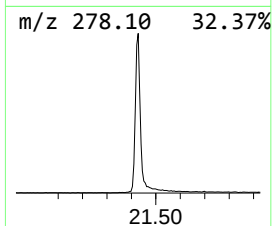
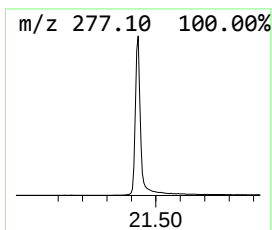
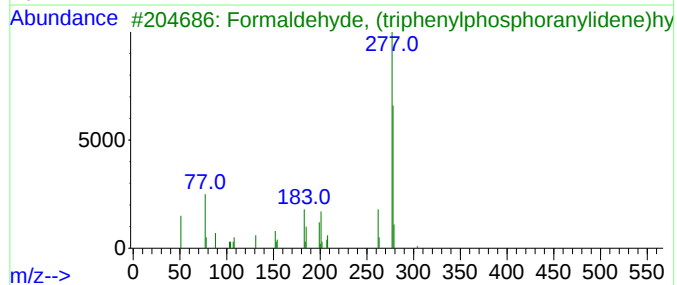
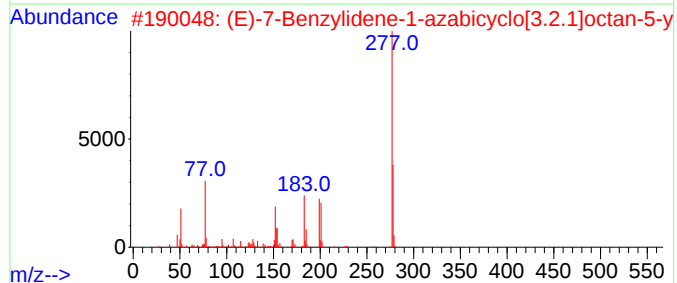
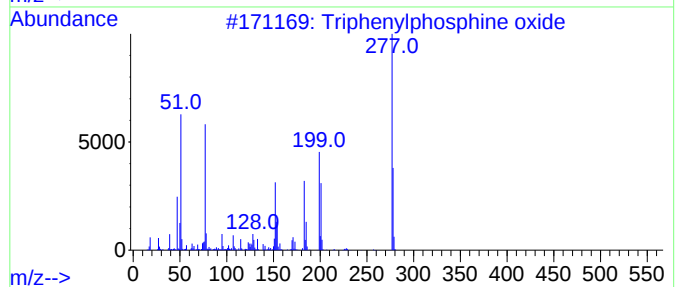
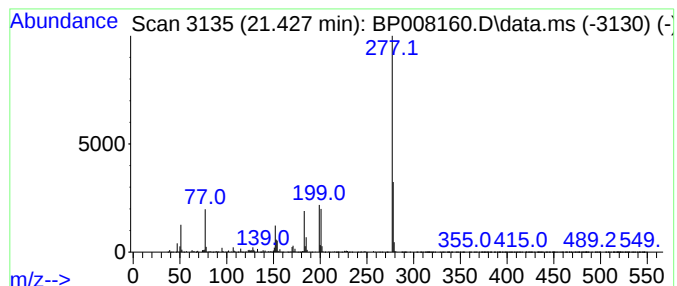
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.427	31.08 ng	1869730	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008160.D
Acq On : 30 Nov 2021 16:08
Operator : CG/JU
Sample : M4848-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PSC124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.011	30.2	ng	891541	1	7.805	589561	20.0
2-Pentanone, 4-...	4.928	9.6	ng	282672	1	7.805	589561	20.0
Ethanol, 2-(2-b...	10.399	2.5	ng	90440	2	10.599	737583	20.0
.beta.-D-Glucop...	14.304	2.4	ng	103659	3	14.445	852808	20.0
Cyclohexadecane	21.033	3.6	ng	216920	5	21.310	1203010	20.0
Diethylene glyc...	21.086	2.6	ng	156300	5	21.310	1203010	20.0
Triphenylphosph...	21.427	31.1	ng	1869730	5	21.310	1203010	20.0